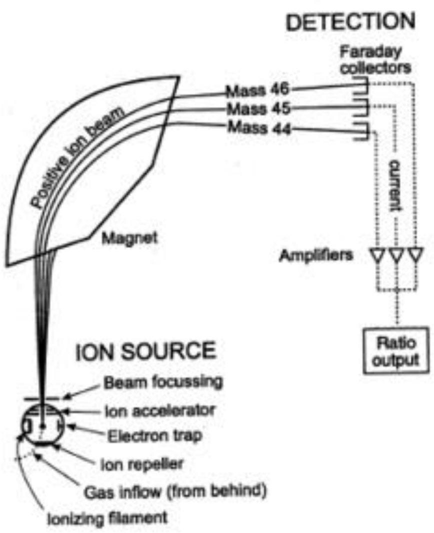
Percent Composition of Compounds

The formula of a compound tells us the numbers of atoms of each element in a unit of the compound. When compounds are used in a research laboratory, verification of the purity of compounds must be made. Such tests can be run using a mass spectrometer which splits up compounds depending on their atomic masses.



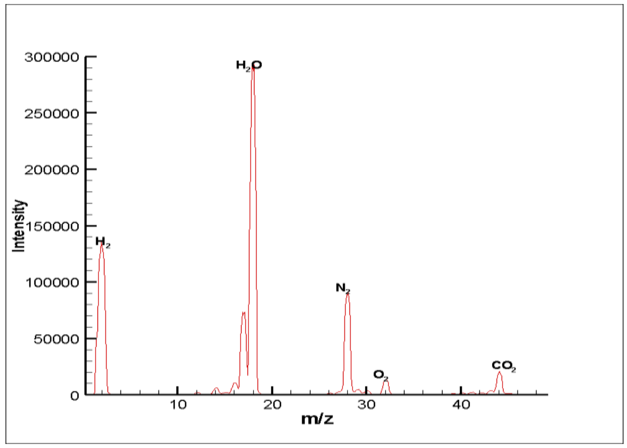


Diagram of a Mass Spectrometer

Output data from a Mass Spectrometer

From the formula of a compound we can calculate the percent of the total mass of the compound is contributed by each element. The ***percent composition by mass*** is the percent by mass of each element in a compound. Percent composition is obtained by dividing the mass of each element in 1 mole of the compound by the molar mass of the compound and multiplying by 100 percent. In the following equation, n is the number of moles of the element in 1 mole of the compound. In one mole of H_2O_2 there are 2 moles of H atoms and 2 moles of O atoms.

$$\text{\% composition of an element} = \frac{\text{n x molar mass of element}}{\text{molar mass of compound}} \text{ x 100\%}$$

Percent composition of H_2O_2 is calculated as follows:

$$\%H = \frac{2 \text{ x } 1.00 \text{ g H}}{34.00 \text{ g } H_2O_2} \text{ x 100\% = 5.88 \% H}$$

$$\%O = \frac{2 \text{ x } 16.00 \text{ g O}}{34.00 \text{ g } H_2O_2} \text{ x 100\% = 94.12 \% O}$$

The sum of the percentages, 5.88% + 94.12% = 100%. It will often be slightly less than or greater than 100% due to rounding.

Finding the Empirical Formulas

If we would like to determine the empirical formula of a compound, given the percentage of each element in the compound, we can do so as in the following example.

Ascorbic acid (vitamin C) cures scurvy. It is composed of 40.92 percent carbon (C), 4.58 percent hydrogen (H), and 54.50 percent oxygen (O) by mass. Determine its empirical formula.

Strategy: In a chemical formula, the subscripts represent the ratio of the number of moles of each element that combine to form one mole of the compound. How can we convert from mass percent to moles? If we assume an exactly 100 g sample of the compound, we then know the mass of each element in the 100 g sample.

Solution: If we have 100 g of ascorbic acid, then each percentage can be converted directly to grams. In this sample, there will be:

$$n_C = 40.92\ \%\ C \rightarrow 40.92\ g\ C \times \frac{1\ mol\ C}{12.0\ g\ C} = 3.41\ mol\ C$$

$$n_H = 4.58\ \%\ H \rightarrow 4.58\ g\ H \times \frac{1\ mol\ H}{1.00\ g\ H} = 4.58\ mol\ H$$

$$n_O = 54.50\ \%\ O \rightarrow 54.50\ g\ O \times \frac{1\ mol\ O}{16.0\ g\ O} = 3.41\ mol\ O$$

Thus, we have the formula: $C_{3.41}H_{4.48}O_{3.41}$ which gives us the identity and the mole ratios of atoms present. However, chemical formulas are written in whole numbers. Try to convert whole numbers by dividing all the subscripts by the smallest subscript (3.41):

$$C: \frac{3.41}{3.41} = 1 \qquad H: \frac{4.54}{3.41} = 1.33 \qquad O: \frac{3.41}{3.41} = 1$$

We need 1.33 to be a full integer, at this point our formula is $CH_{1.33}O$. We can find an integer for H by trial-and-error:

1.33 x 1 = 1.3
1.33 x 2 = 2.7
1.33 x 3 = 4.0

We then multiply each of the elements by 3, going from $CH_{1.33}O$ to $C_3H_4O_3$ and as you can see the subscripts are reduced to the smallest possible whole numbers. Our final empirical formula is:

$C_3H_4O_3$

Examples from: Chang, Raymond, *General Chemistry,* 7th edition